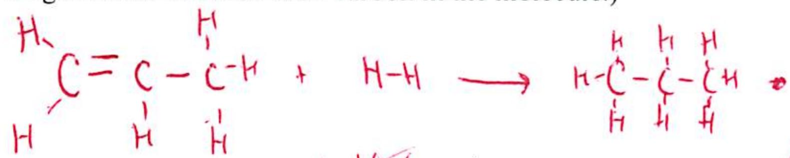
Using Bond Energies to Calculate Heats of Reaction

1. Hydrogenation reactions, which involve the addition of H_2 to a molecule, are widely used in industry to transform one compound into another. For example, 1-propene (C_3H_6) is converted to propane (C_3H_8) by addition of H_2. Use bond energy values to estimate the enthalpy change for this hydrogenation reaction. (Note: To do this problem you must know the structure of each molecule. For 1-propene, there is a double bond between the first two carbons. Everywhere else has a single bond. For propane, there are only single bonds between each carbon in the molecule.)



ΔH = [~~6mol (C-H)~~ + 1mol (C=C) + 1mol (H-H)] − [2 mol (C-H) + 1 mol (C-C)]   (+1mol C-C)

1mol (614 kJ/mol) 1mol (432 kJ/mol) − [2mol (413 kJ/mol) + 1mol 347 kJ/mol] = -127 kJ/mol

2. Estimate the heat of combustion of propane from the previous problem using bond energy values. Then use heat of formation values to calculate the actual heat of combustion for the reaction. Is there much difference between each value?

$C_3H_{8(g)} + 5O_{2(g)} \rightarrow 3CO_{2(g)} + 4H_2O_{(g)}$

C-C-C

ΔH = [8mol (C-H) + 2 C-C + 5mol (O=O)] − [6mol (C=O) + 8mol (O-H)]

= 8mol (413 kJ) + 2(347) + 5mol (495 kJ) − [6mol (799 kJ) + 8mol (467 kJ)]

ΔH = -2057 kJ/mol

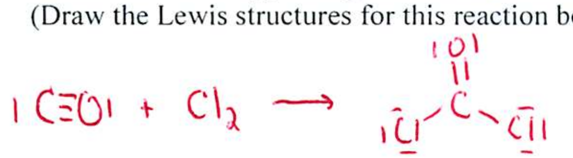
ΔH_f = 4(-242 kJ) + 3(-393.5 kJ) − (-104 kJ [illegible])

= -2044.5 kJ

13 kJ off

Yes But based on ~~[illegible]~~ and their according enthalpy changes I can see why.

3. Phosgene, Cl_2CO, is a highly toxic gas that was used as a weapon in WWI. Using bond energy values, estimate the enthalpy change for the reaction of carbon monoxide and chlorine to produce phosgene. (Draw the Lewis structures for this reaction before calculating the bond energy values.)



ΔH = [1mol (C≡O) + 1mol (Cl-Cl)] − [2mol (C-Cl) + 1mol C=O]

1mol (1072 kJ/mol) + 1mol (239 kJ/mol) − (2mol (339 kJ/mol) + 1mol (745 kJ)) = -112 kJ

4. Oxygen difluouride gas is very reactive producing oxygen gas and hydrogen fluoride gas when coming in contact with water vapor. This reaction is also quite exothermic releasing 318 kJ of energy per mole of oxygen difluoride. Using bond energies, calculate the bond energy of an O—F bond in oxygen difluoride.

2mol (O-F) + 2mol (H-O) − [1mol (O=O) + 2mol (H-F)] = -318 kJ

2x + 2mol (467 kJ) − [1mol (495 kJ) + 2mol (565 kJ)] = -318 kJ

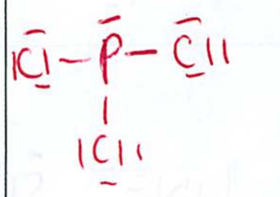
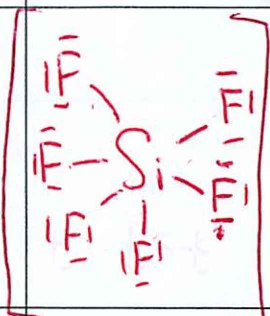
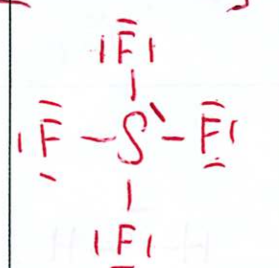
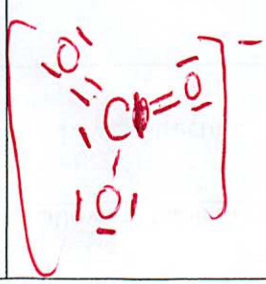
2x = 373

x = 186.5 ≈ 187 kJ   on table its 190 so it agrees w/ s.f.

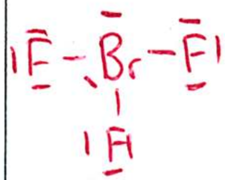
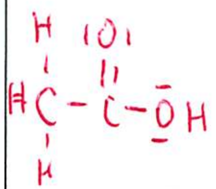
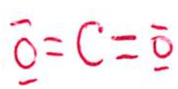
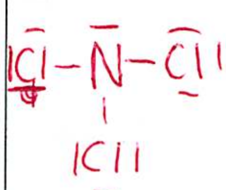
Lewis Structures Sheet

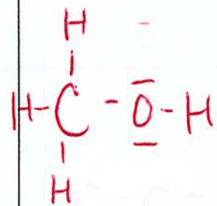
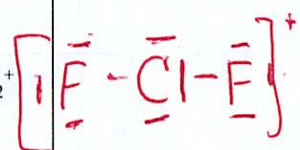
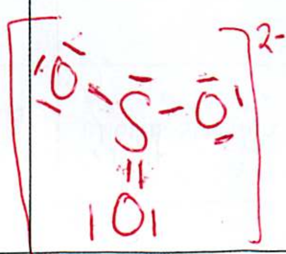
Complete the following table. You will not be able to complete this all at once.

Name/ Formula	Lewis Structure	Polar Bonds in Molecule? If so, which ones?	Polar Molecule (Y/N)	# bonding pairs of e^- on central atom	# non-bonding e^- pairs on central atom	Molecular Geometry	Hybridization	# of σ-bonds	# of π-bonds
H_2S	H—S—H	yes S—H	Y	2	2	Bent	sp^3	2	0
BeF_2	F -Be-F	yes Be—F	N	2	0	linear	sp	2	0
SCN^-	$[S-C\equiv N]^-$	yes S—C C—N	ion	4	0	linear	sp	2	2
BF_3		B—F	N	3	0	trigonal planar	sp^2	3	0

Name/ Formula	Lewis Structure	Polar Bonds in Molecule? If so, which ones?	Polar Molecule (Y/N)	# bonding pairs of e⁻ on central atom	# non-bonding e⁻ pairs on central atom	Molecular Geometry	Hybridization	# of σ-bonds	# of π-bonds
PCl_3		Yes P–Cl	Y	3	1	trigonal pyramidal	sp^3	3	0
SiF_6^{2-} 24e⁻		Yes Si–F	N	6	0	Octahedral	d^2sp^3	6	0
SF_4 17		Yes S–F	y	4	1	See Saw	dsp^3	4	0
ClO_3^- 13		Yes Cl–O	Ion	5	1	trig pyramidal	d^2sp	3	2

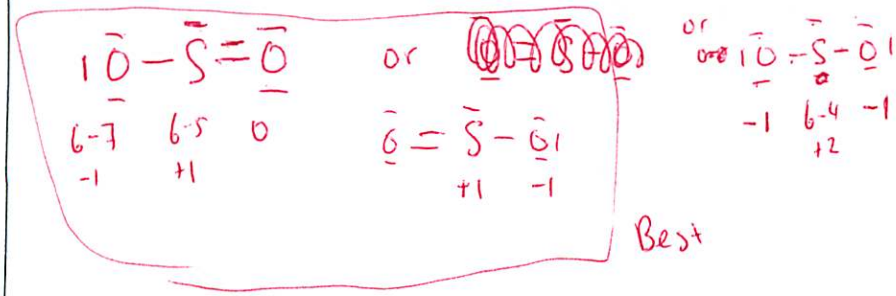
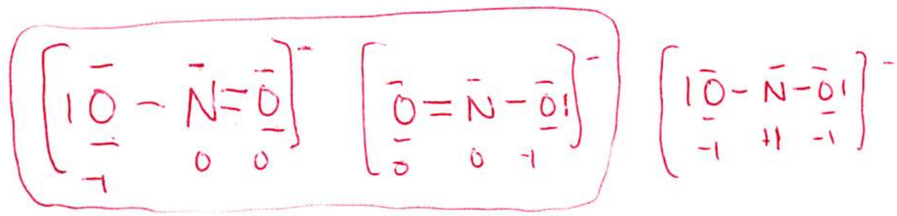
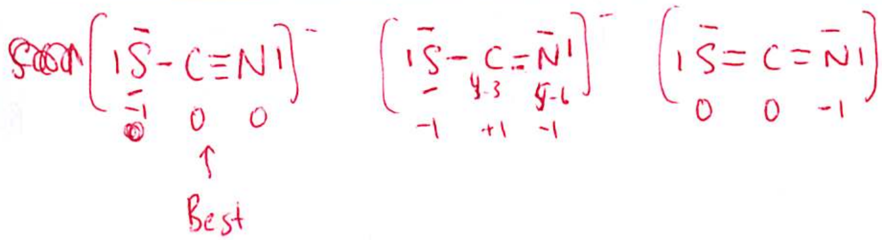
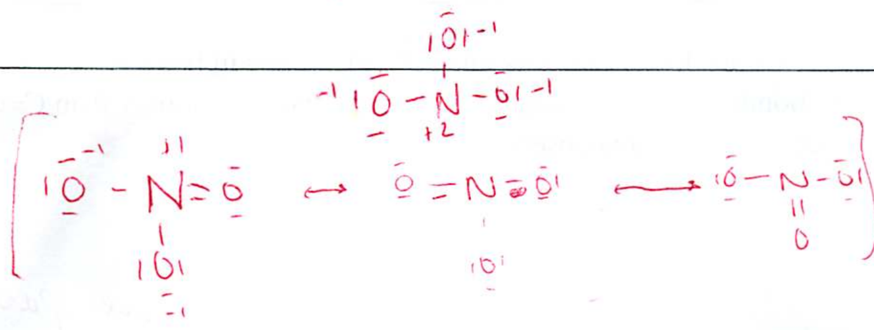
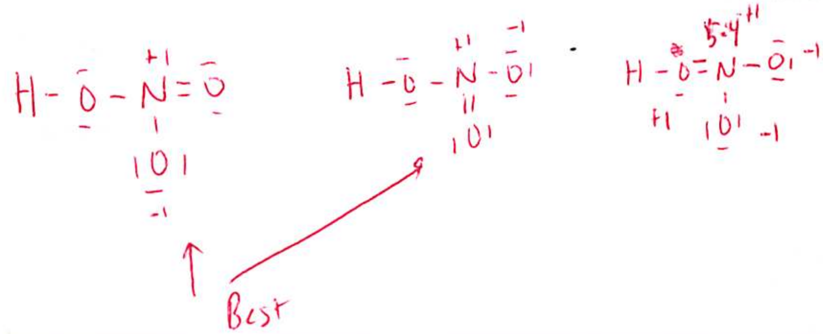
★

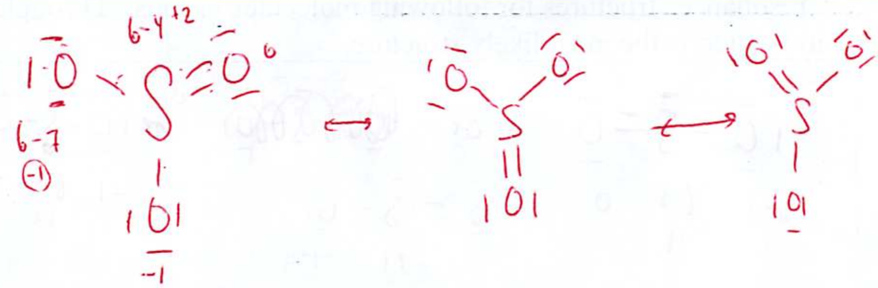
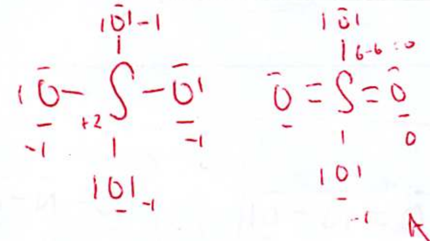
Name/ Formula	Lewis Structure	Polar Bonds in Molecule? If so, which ones?	Polar Molecule (Y/N)	# bonding pairs of e^- on central atom	# non-bonding e^- pairs on central atom	Molecular Geometry	Hybridization	# of σ-bonds	# of π-bonds
BrF_3		Br—F	y	3	2	~~[illegible]~~ Tshaped	dsp^3	3	0
CH_3COOH		Yes CH, C—O, OH	y	CH_3 - 4 C - 4 O - 2	→ 0 → 0 → 2	→ tetrah → trigplan → Bent	sp^3 sp^2 → sp^3	4 3 2	0 1 0
CO_2		C—O	N	4	0	linear	sp	2	2
NCl_3		~~[illegible]~~ Yes No ~~[illegible]~~	y	3	1	trigonal pyramidal	sp^3	3	0

Name/ Formula	Lewis Structure	Polar Bonds in Molecule? If so, which ones?	Polar Molecule (Y/N)	# bonding pairs of e⁻ on central atom	# non-bonding e⁻ pairs on central atom	Molecular Geometry	Hybridization	# of σ-bonds	# of π-bonds
CH_3OH		CH, OH, C–O	y	C - 4 O - 2	0 2	tetrahedra Bent	sp^3 sp^3	4 2	0 0
ClF_2^+ 10 pair		y Cl–F	Ion	2	2	Bent	sp^3	2	0
CS_2		y C–S	N	4	0	linear	sp	2	2
SO_3^{2-} @13		y S–O	Ion	4	~~2~~	trigonal ~~planar~~ pyramidal	dsp^2	3	1

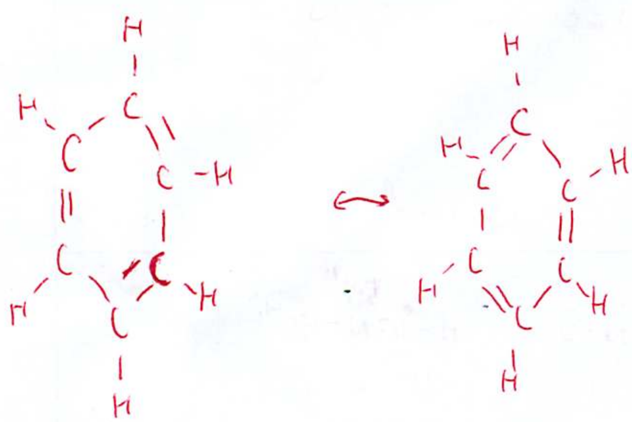
Resonance

Draw the possible resonance structures for following molecules or ions. Through formal charges on atoms, determine which is the most likely structure.

SO_2 9 pairs	
NO_2^- 9 pair	 Best
SCN^-	
NO_3^- 24 12e	 all equal.
HNO_3	

SO_3	
SO_4^{2-}	 More Stable
O_3	 Both even

Use the concept of resonance to explain why all six C—C bonds in benzene, C_6H_6, are equal in length. These C—C bonds are shorter than C—C single bonds, but longer than C=C double bonds. Use resonance to explain this observation.



all Bonds have partial single and double bond characteristics so it shortens the bonds but keeps them longer than single Bonds